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Low-temperature phonon dynamics of a classical compressible Heisenberg chain

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Abstract. A low-temperature calculation of the influence of the anharmonicity of the phonons on the dynamic structure factor is made for a compressible Heisenberg system. The anharmonicity is caused by the coupling of phonons and spins. The memory function of the displacement relaxation function is calculated to lowest order in the temperature. Only two-magnon processes are found to contribute to the memory function in this limit. The displacement relaxation function turns out to be very simple. The collision processes can lead to a second resonance. In two limits, the results are compared with the results of a continued fraction approximation. The qualitative agreement is good.

1. Introduction

In a previous paper (Fivez *et al* 1980) we presented a detailed study of the phonon dynamics in a compressible Heisenberg chain (CHC). As a starting point we took the continued fraction expansion of the displacement relaxation function. A four-pole approximation was then used. Here we take up the subject again from a different point of view. We use a method, originally due to Reiter and Sjölander (Reiter and Sjölander 1980, Reiter 1980), that yields exact results in the low-temperature limit. The approach is based on a low-temperature expansion of the memory function, retaining only the lowest-order non-vanishing term. We use a slightly different but equivalent formulation of their approach.

We find it interesting to study the phonons in the CHC again within this theory for the following reasons. First, the truncation approximation for the continued fraction that was used is based on the assumption that the memory function contains no slow processes (De Raedt and De Raedt 1977). At low temperatures however the memory function turns out to have a very slow and oscillatory time dependence and the approximation becomes questionable. Therefore it seems worthwhile to compare the results of the four-pole approximation with the results of a low-temperatue theory (LTT). Second, the present study sheds light on features of the LTT that were not present in the case of the rigid Heisenberg chain (RHC) (Reiter *et al* 1980). The memory function in the LTT has poles and a cut-off. The crucial point is that for the RHC the spinwave peak is always situated below poles and cut-off. For the phonon resonance of the CHC this is not always true. We find a displacement relaxation function of strikingly simple functional form

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that has a peculiar parameter dependence. Thirdly, the theory not only demonstrates what kind of interaction processes are responsible for the phonon relaxation to lowest order in the temperature, but also how they cause the relaxation. In this way the mechanism of the non-linear processes becomes more transparent. Last but not least, a treatment of the dynamics of a coupled system that yields all frequency moments exact up to first order in the temperature is interesting in its own right.

The plan of the paper is as follows. In § 2 we define the model. The basic theory is then given. The harmonic approximation of the model is discussed. In § 3 we give the results for the memory function. In § 4 the results are discussed and we compare them with our previous work. The conclusions are summarised in § 5.

2. Model and basic theory

The compressible spin system we consider is described by the Hamiltonian (Fivez *et al* 1980 and references quoted therein)

$$H = H_P + H_S + H_{SP} \tag{2.1a}$$

$$H_P = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{\alpha}{2} \sum_{i=1}^{N-1} (x_{i+1} - x_i)^2 \tag{2.1b}$$

$$H_S = -J \sum_{i=1}^{N-1} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \tag{2.1c}$$

$$H_{SP} = -\varepsilon \sum_{i=1}^{N-1} (x_{i+1} - x_i)\, \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}. \tag{2.1d}$$

The spins are located on a harmonic lattice with an exchange interaction depending linearly on the atom–atom separation. We consider classical spins of unit length.

The quantity we want to calculate is the equilibrium displacement correlation function

$$C(q, z) = -i \int_0^\infty \mathrm{d}t \exp(\mathrm{i}zt)\, C(q, t); z = \omega + \mathrm{i}\varepsilon, \tag{2.2a}$$

where

$$C(q, t) \equiv (x_q(t), x_q) = (x_q, \exp(-\mathrm{i}Lt)\, x_q). \tag{2.2b}$$

Here we use the notation

$$(A, B) = \langle (A - \langle A \rangle)^+ (B - \langle B \rangle) \rangle, \tag{2.3}$$

and the Liouville operator is given by

$$LA = [H, A] \tag{2.4}$$

Following Mori (1965) we can write

$$C(q, z) = C(q, t = 0) \left(z - \frac{\langle \omega^2 \rangle_q}{z + \Sigma_q(z)} \right)^{-1} \tag{2.5}$$

where $\langle\omega^2\rangle_q$ is the second frequency moment given by

$$\langle\omega^2\rangle_q = \frac{(Lx_q, Lx_q)}{(x_q, x_q)} \tag{2.6}$$

which can be calculated rigorously by means of the transfer operator method (Fivez *et al* 1980).

In the low-temperature limit we have

$$\langle\omega^2\rangle_q = 2(\alpha/m)(1 - \cos q)(1 - \tilde{T}) \tag{2.7a}$$

$$\tilde{T} = \gamma T/J(1 + |\gamma|)^2 \tag{2.7b}$$

$$\gamma = \varepsilon^2/\alpha J. \tag{2.7c}$$

$\Sigma_q(z)$ is the memory function defined by

$$\Sigma_q(z) = -(Lx_q, Lx_q)^{-1}(QL^2x_q, (z - QLQ)^{-1}QL^2x_q), \tag{2.8a}$$

where Q is the projection operator which projects onto the non-secular variables and is defined by

$$QB_q = B_q - \frac{(Lx_q, B_q)}{(Lx_q, Lx_q)}Lx_q - \frac{(x_q, B_q)}{(x_q, x_q)}x_q. \tag{2.8b}$$

In time space the memory function reads

$$\Sigma_q(t) = -(Lx_q, Lx_q)^{-1}M_q(t) \tag{2.9a}$$

$$M_q(t) = (QL^2x_q, \exp(-\mathrm{i}QLQt)QL^2x_q). \tag{2.9b}$$

In principle the exact calculation of Σ_q is prohibitively complicated. However, as $T \to 0$ Σ_q vanishes proportional to T because the phonons decouple from the spin fluctuations and consequently the system becomes harmonic (Fivez *et al* 1980). If we content ourselves with a displacement correlation function that has frequency moments correct up to first order in T, it follows that we can limit ourselves to the calculation of the lowest-order term of equation (2.9). Reiter and Sjölander (1980) showed that in order to calculate this lowest-order term we can replace QLQ in equations (2.8) and (2.9) by the normal time evolution operator L. More specifically, we can write

$$M_q(t) = (QL^2x_q, \exp(-\mathrm{i}Lt)QL^2x_q) + \mathrm{O}(T^3). \tag{2.10}$$

Their argument is formulated in time space. The same result can also be obtained directly in frequency space. Defining

$$\Lambda_q(z) = -(Lx_q, Lx_q)^{-1}(QL^2x_q, (z - L)^{-1}QL^2x_q), \tag{2.11}$$

one can derive the exact relation

$$(z^2 - \langle\omega^2\rangle_q)\Sigma_q(z) = (z^2 - \langle\omega^2\rangle_q)\Lambda_q(z) + z\Lambda_q(z)\Sigma_q(z). \tag{2.12}$$

Now both Λ_q and Σ_q vanish proportional to T and hence

$$\Sigma_q(z) = \Lambda_q(z) + \mathrm{O}(T^2). \tag{2.13}$$

Strictly speaking, equation (2.13) only holds when the lowest-order term of $\Lambda_q(z)$ is not too large. However, if $\Lambda_q(z)$ has singularities at some frequencies we cannot claim to have an exact result. The result (2.13) is however exact to the extent that it reproduces

all the frequency moments of Σ_q exact to lowest non-vanishing order in T. The advantage of equation (2.10) is that we can use the harmonic approximation for the evaluation of the lowest-order term. This harmonic approximation is based on the Holstein–Primakoff transformation. A justification of the use of this transformation has been given by Reiter (1980). For the ferromagnet we write

$$S_i^z = 1 - \tfrac{1}{2}S_i^- S_i^+ \tag{2.14a}$$

$$S_i^\pm = S_i^x \pm \mathrm{i}\, S_i^y \tag{2.14b}$$

and after Fourier transformation we find

$$H = \sum_q \frac{p_q p_{-q}}{2m} + \alpha \sum_q (1 - \cos q)\, \Delta x_q \Delta x_{-q} + \tfrac{1}{2} \sum_q \omega(q)\, S_q^- S_{-q}^+, \tag{2.15a}$$

where

$$\Delta x_q = (x - \langle x \rangle)_q \tag{2.15b}$$

$$\omega(q) = 2J(1 + \gamma)\,(1 - \cos q), \tag{2.15c}$$

and where the ground state energy has been omitted. Consequently,

$$\langle S_q^+ S_{-q}^- \rangle = \frac{2T}{\omega(q)} \tag{2.16}$$

$$S_q^\pm(t) = \exp(\mp \mathrm{i}\omega(q)t)\, S_q^\pm. \tag{2.17}$$

For the antiferromagnet we write

$$S_i^z = (-1)^i\,(1 - \tfrac{1}{2}S_i^- S_i^+), \tag{2.18}$$

combined with equation (2.14*b*). Again we find the Hamiltonian (2.15*a*) but now we have

$$\omega(q) = 2|J|(1 + |\gamma|)\,(1 + \cos q). \tag{2.19}$$

It follows that now

$$S_q^\pm(t) = \cos(\Omega(q)t)\, S_q^\pm \mp \mathrm{i}\left(\frac{1 - \cos q}{1 + \cos q}\right)^{1/2} \sin(\Omega(q)t)\, S_{q-\pi}^\pm, \tag{2.20a}$$

where

$$\Omega(q) = \left(\omega(q)\,\omega(q - \pi)\right)^{1/2} = 2|J|(1 + |\gamma|)\,|\sin q\,|. \tag{2.20b}$$

Equation (2.16) remains unchanged. Our general scheme to calculate equation (2.10) is then as follows. Use the exact Liouville operator L to calculate $L^2 x_q$. Then expand $L^2 x_q$ in the normal coordinates Δx_q, S_q^+ and S_q^- using the Holstein–Primakoff transformation and retain only linear and quadratic terms. The Q operator then erases the terms linear in Δx_q. Then use the harmonic time evolution and calculate the expectation values using the formulas (2.16) and (2.15*c*) or (2.19).

To close this section, we briefly discuss another procedure. Following Mori (1965), we can equally well write instead of equation (2.5)

$$C(q, z) = C(q, t = 0)\left(z - \frac{\langle \omega^2 \rangle}{z - \Delta_2^2/[z + T_q(z)]}\right)^{-1}, \tag{2.21}$$

where

$$\Delta_2^2(q) = \langle\omega^4\rangle_q/\langle\omega^2\rangle_q - \langle\omega^2\rangle_q \tag{2.22}$$

can be calculated exactly (Fivez *et al* 1980). $T_q(z)$ is now given by

$$T_q(z) = -(A_q, A_q)^{-1}(QL^3x_q, (z - QLQ)^{-1}QL^3x_q), \tag{2.23a}$$

where

$$A_q = L^2x_q - \langle\omega^2\rangle_q x_q, \tag{2.23b}$$

and $\dot{Q}$ is defined by

$$QB_q = B_q - \frac{(x_q, B_q)}{(x_q, x_q)}x_q - \frac{(Lx_q, B_q)}{(Lx_q, Lx_q)}Lx_q - \frac{(A_q, B_q)}{(A_q, A_q)}A_q. \tag{2.23c}$$

As $\Delta_2^2 \propto T$ in the low-temperature limit we only need the $T = 0$ result for $T_q(z)$ in order to get the same kind of approximation for $C(q, z)$ as before. In $T_q(z)$, however, we may not replace QLQ by L to lowest order in T. This difficulty can be circumvented in the following way.

Defining

$$\gamma_q = -(A_q, A_q)^{-1}(QL^3x_q, (z - L)^{-1}QL^3x_q), \tag{2.24}$$

one has the exact relation

$$z\left(z^2 - \frac{\langle\omega^4\rangle_q}{\langle\omega^2\rangle_q}\right)\gamma_q(z) + (z^2 - \langle\omega^2\rangle_q)\gamma_q(z)T_q(z) = z\left(z^2 - \frac{\langle\omega^4\rangle_q}{\langle\omega^2\rangle_q}\right)T_q(z). \tag{2.25}$$

For $T = 0$ this becomes

$$T_q(z, T = 0) = \frac{z\gamma_q(z, T = 0)}{z - \gamma_q(z, T = 0)}, \tag{2.26}$$

where γ_q may again be calculated in the harmonic approximation. The same scheme as for the calculation of equation (2.10) can then be used.

We will show that both procedures lead to the same result for the correlation functions, showing the consistency of the theory.

3. The memory function

Let us first focus on equation (2.10). Consider the ferromagnet. Following our general scheme, we find

$$QL^2x_q = 2(\varepsilon/m)\sin\frac{q}{2}N^{-1/2}\sum_k\left(\cos k - \cos\frac{q}{2}\right)S^-_{q/2-k}S^+_{q/2+k}. \tag{3.1}$$

This yields, using equations (2.14–17)

$$(QL^2x_q, e^{-iLt}QL^2x_q) = \frac{4\varepsilon^2}{m^2}\sin^2\frac{q}{2}\frac{T^2}{J^2(1+\gamma)^2}$$
$$\times\frac{1}{N}\sum_k\exp[i(\omega(k - q/2) - \omega(k + q/2))t]. \tag{3.2}$$

Using the formula

$$\lim_{N\to\infty} \frac{1}{N} \sum_k \cos(a \sin k\, t) = J_0(at), \tag{3.3}$$

where J_0 is the Bessel function of order zero, one finds

$$\Sigma_q(t) = -\Delta_2^2 J_o(at), \tag{3.4}$$

and consequently

$$\Sigma_q(z) = i\Delta_2^2/(a^2 - z^2)^{1/2}. \tag{3.5}$$

Here a is defined by

$$a(q) = 4J(1 + \gamma)\,|\sin q/2\,|, \tag{3.6}$$

Δ_2^2 is defined in equation (2.22) and use has been made of the low-temperature result

$$\Delta_2^2 = \frac{2\alpha}{m}(1 - \cos q)\,\tilde{T} + O(T^2). \tag{3.7}$$

For the antiferromagnet we must use equations (2.18–20) but the result turns out to be the same, when J and γ are replaced by their absolute value. Remark that $\Sigma_q(t)$ is essentially the self-correlation function of the spin energy density at zero temperature (De Raedt and De Raedt 1980). This is so because in the Hamiltonian (2.1) the displacements are coupled with the spin energy.

Now the energy relaxation at $T = 0$ is independent of the sign of the spin–spin interaction (De Raedt and De Raedt 1980). However, for finite T the spin energy relaxation function is different for ferro- and antiferromagnets (De Raedt *et al* 1981). Consequently, the independence of the phonon function of the sign of J will not persist at higher temperatures.

Now consider equation (2.21). Then we have to calculate (2.26). Take again the ferromagnet. Following the general scheme we find

$$QL^3x_q = \frac{4\varepsilon J(1+\gamma)}{m} \sin\frac{q}{2} N^{-1/2} \sum_k S^-_{q/2-k} S^+_{q/2+k} (\cos k - \cos q/2) \times [\cos(k + q/2) - \cos(k - q/2)]. \tag{3.8}$$

Making use of equations (2.14–17), equation (2.24) and the integral representation of the Bessel functions one finds

$$\gamma_q(z) = \frac{iz^2}{(a^2 - z^2)^{1/2}} + z. \tag{3.9}$$

Combining equations (2.21), (2.26) and (3.9) we finally obtain

$$C(q, z) = C(q, t = 0) \Big/ \left(z - \frac{\langle\omega^2\rangle_q}{z - \Delta_2^2 i/(a^2 - z^2)^{1/2}}\right). \tag{3.10}$$

Though the calculation uses equations (2.18–20), again the same results (3.9) and (3.10) are recovered for the antiferromagnet. Comparing equation (3.10) with (2.5) combined with (3.5), we see that the approaches (2.5) and (2.21) lead to exactly the same result. It is possible to prove generally the equivalence of both approaches within the scheme

for the calculation of the memory functions. This proves that the harmonic treatment leads to consistent results.

4. Discussion

The memory function given by equation (3.5) diverges for $z = a$ (equation (3.6)). This is a consequence of a divergence in the two-magnon density of states

$$n = \left| \frac{\mathrm{d}k}{\mathrm{d}\Omega_-} \right|, \tag{4.1}$$

with

$$\Omega_- = \omega\left(k + \frac{q}{2}\right) - \omega\left(k - \frac{q}{2}\right). \tag{4.2}$$

This is easily understood as follows. Following equation (3.2), two processes contribute to the memory function. In the first process a magnon of wavevector $k - q/2$ is absorbed and a magnon with wavevector $k + q/2$ is emitted. Another possibility is the decay of a magnon $k + q/2$ into a magnon $k - q/2$. The possible processes are sketched in figure 1. At the k vector for which n diverges there are infinitely many possible processes with the same energy gain or loss Ω_- and consequently the relaxation is very large at this frequency Ω_-.

The quantity of interest is the dynamic structure factor $C_q(\omega)$, which is minus the imaginary part of $C(q, z)$ and is given by

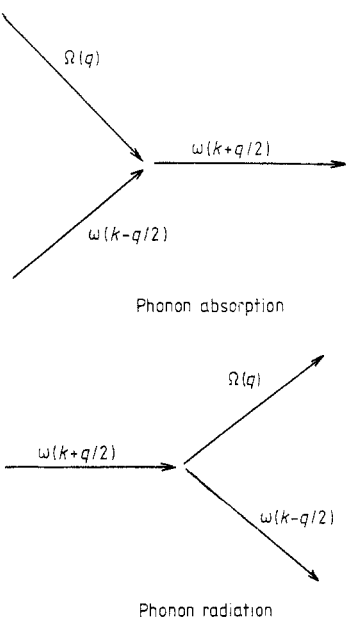

Figure 1. The interaction processes that are responsible for the phonon damping. ω denotes the magnon frequency. Ω, q respectively denote the energy and wavevector gain or loss in the process. There are absorption and radiation processes.

$$C_q(\omega) = \frac{\langle\omega^2\rangle_q \Sigma''_q(\omega)}{(\omega^2 - \langle\omega^2\rangle_q + \omega\Sigma'_q(\omega))^2 + (\omega\Sigma''_q(\omega))^2}, \tag{4.3}$$

where C_q has been normalised such that

$$\frac{1}{\pi}\int_{-\infty}^{\infty} C_q(\omega)\,\mathrm{d}\omega = 1. \tag{4.4}$$

Σ'_q and Σ''_q are the real and imaginary part of $\Sigma_q(\omega + i\varepsilon)$ $(\varepsilon \to 0^+)$. From equation (3.5)

$$\Sigma'_q(\omega) = 0; \qquad 0 < \omega \leqslant a, \tag{4.5a}$$
$$\Sigma'_q(\omega) = -\Delta_2^2/(\omega^2 - a^2)^{1/2}; \qquad \omega > a, \tag{4.5b}$$
$$\Sigma''_q(\omega) = \Delta_2^2/(a^2 - \omega^2)^{1/2}; \qquad 0 < \omega < a, \tag{4.5c}$$
$$\Sigma''_q(\omega) = 0; \qquad \omega \geqslant a. \tag{4.5d}$$

Remark that we chose the sign of the square root such that

$$\Sigma'' \geqslant 0, \tag{4.6a}$$

$$\Sigma' \leqslant 0 \text{ for } \omega > a. \tag{4.6b}$$

Relation (4.6*a*) is the damping condition and equation (4.5*b*) follows from it through the Kramers–Kronig relations. Following equations (4.5) we must distinguish two cases, $|\omega| \gtrless a$. For $|\omega| < a$ we have to combine equations (4.3) and (4.5*a*, *c*). For $|\omega| > a$ equations (4.3) and (4.5*b*, *d*) give

$$C_q(\omega) = \pi\langle\omega^2\rangle_q \sum_{|\omega_i|>a} \delta(\omega - \omega_i) \Big/ \left|\omega_i \frac{\mathrm{d}f}{\mathrm{d}\omega}(\omega_i)\right|, \tag{4.7a}$$

where we defined

$$f(\omega) = \omega^2 - \langle\omega^2\rangle_q + \omega\Sigma'_q(\omega), \tag{4.7b}$$

and ω_i are the zeros of $f(\omega)$.

Defining

$$B^2 = \frac{a^2(q)}{\langle\omega^2\rangle_q} = 4J^2 m(1 + |\gamma|)^2 (1 + \tilde{T})/\alpha, \tag{4.8}$$

measuring the frequency in units of a and the structure factor in units of $1/a$ we find

$$C_q(\omega) = \theta(1 - |\omega|)\,\tilde{T}(1 - \omega^2)^{1/2}/[(1 - \omega^2)\,(\omega^2 B^2 - 1)^2 + \omega^2\tilde{T}^2]$$
$$+ \theta(|\omega| - 1)\frac{\pi}{B^2}\sum_i \delta(\omega - \omega_i) \Big/ \left|\omega_i \frac{\mathrm{d}f}{\mathrm{d}\omega}(\omega_i)\right|. \tag{4.9}$$

Equation (4.9) depends only on two parameters, $\tilde{T}$ and B. Neither B nor $\tilde{T}$ depends on the wavevector q. Hence the scaled structure factor (4.9) is independent of q. This very important result is due to the coincidence that the cut-off frequency $a(q)$ of the collision processes has the same q-dependence as the phonon dispersion. Equation (4.9) must be interpreted as follows. Phonon processes of wavevector q with a frequency lower than $a(q)$ are damped by two-magnon processes. All processes with a frequency higher than $a(q)$ are undamped because the frequency does not fit the energy gain or loss of any possible two-magnon process of figure 1. Indeed, $a(q)$ is the maximum of Ω_- defined in equation (4.2).

In the discussion of equation (4.9), the part of the spectrum below $\omega = 1$ causes no difficulties. The higher part, however, requires a knowledge of the zeros of $f(\omega)$, equation (4.7*b*), which are the solutions of a third-order equation. Let us distinguish between three different regimes depending on the value of B.

4.1. $B > 1$

Here the phonon frequency is sufficiently lower than the highest frequency of a collision process. Here the structure factor (4.9) essentially becomes a pair of Lorentz lines at the frequencies

$$\omega = \pm 1/B \tag{4.10}$$

with a half width at half maximum given by

$$\Delta_q = \frac{\tilde{T}}{2B(B^2 - 1)^{1/2}}. \tag{4.11}$$

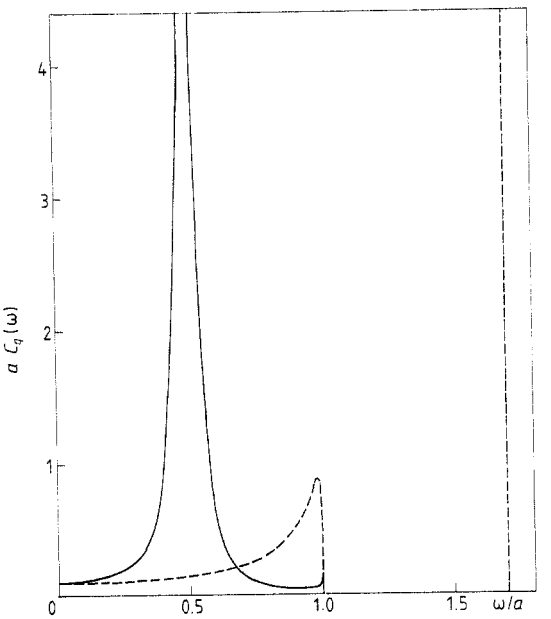

Figure 2. The dynamic structure factor in the two different regimes: $B = 2$ (——) and $B = 2/3$ (– – –). The scaling factor $a(q)$ is given by equation (3.6). The scaled structure factor is independent of q. For $B = 2/3$ the delta function has a weight of approximately 80% of the total area. $\tilde{T} = 0.1$.

There is an additional peak of very low weight at $\omega \approx 1$. The part of the spectrum for $\omega > 1$ is of negligible weight. Figure 2 shows a typical plot of the structure factor. The dependence on $\tilde{T}$ is not shown. Its only effect is to change the width of the Lorentz lines and the weight of the small peak at $\omega \approx 1$.

4.2. $B < 1$

Now the undamped part of the spectrum is dominant. It consists of a pair of delta peaks at

$$\omega = \pm \frac{1}{B}\left(1 + \frac{\tilde{T}}{(1 - B^2)^{1/2}}\right). \tag{4.12}$$

In addition, there are resonances of low weight at $\omega \approx \pm 1$. The relative weight of these resonances is given by

$$w = x/(1 - x), \tag{4.13a}$$

where x is defined as

$$x = \tilde{T}(1 - B^2/2)/(1 - B^2)^{3/2}. \tag{4.13b}$$

Although this is relatively unimportant it is detectable because the dominant peaks are very narrow and hence the second resonances are not lost in the tails of the main resonance. Figure 2 also depicts the structure factor in this regime. Again the T dependence is omitted. It merely affects the weight of the second resonance.

4.3. $B \approx 1$

In this case the phonon frequency is close to the cut-off frequency and the whole weight of the spectrum is now concentrated in a narrow region around the cut-off. For $B \gtrsim 1$ the lines are no longer Lorentzian but have an asymmetric shape and the undamped part of the spectrum is no longer negligible. For $B = 1$ the separation between the cut-off and the delta function is proportional to $\tilde{T}^{2/3}$.

We now compare our results with those found previously using a continued fraction approach (Fivez *et al* 1980). For this aim, consider the results of the continued fraction method for $T \approx 0$. At low temperatures narrow lines are observed and therefore it is sufficient to examine the shape near the peak positions. Then the memory function may be evaluated at $\omega = \langle\omega^2\rangle^{1/2}$. For $B \gg 1$ we find

$$\Sigma' \approx 0, \tag{4.14a}$$

$$\Sigma'' \approx \frac{\sqrt{2}\,\tilde{T}a}{B^2}. \tag{4.14b}$$

Comparing this with equations (4.5*a*, *c*) we see that the only difference is that Σ'' is $\sqrt{2}$ times larger. Consequently, the continued fraction gives a Lorentzian line at the same position, $\langle\omega^2\rangle^{1/2}$ unshifted, but with a width $\sqrt{2}$ times as large. For $B \ll 1$ the result reads

$$\Sigma' \approx -a\tilde{T}/B, \tag{4.15a}$$

$$\Sigma'' \approx 0. \tag{4.15b}$$

Comparing with equations (4.5*b*, *d*), we see that the results are identical. In addition to the line at the phonon frequency the continued fraction produces a central peak for $B \ll 1$. This peak is to be compared with the peak at $\omega \approx 1 \ll B$ in the present theory. Of course, the four-pole approximation necessarily smears out such peaks leading to the observed central peak. For $B \approx 1$ no agreement is found between the continued fraction and the present results.

5. Conclusions

The phonon relaxation function of a compressible Heisenberg chain at low temperatures was studied. For this purpose the lowest-order contribution to the memory function was calculated using a prescription that was shown to be consistent. The results are exact to the extent that all frequency moments of the correlation function are given rigorously up to order T. Scaling the frequency and intensity, the structure factor was found to be independent of the wavevector. For some parameter values a second resonance besides the usual phonon peak was observed. This is due to a divergency in the two-magnon density of states.

Our model is confined to nearest-neighbour interactions. The procedure to calculate the memory function is equally well applicable if further-neighbour interactions are included. Obviously the dispersions and hence the divergencies in the two-magnon density of states would change, but qualitatively we do not expect much difference. A practical difficulty would be the exact calculation of the second frequency moment $\langle\omega^2\rangle_q$ up to first order in the temperature, because the transfer operator method can only be applied to the nearest-neighbour case.

Let us also discuss what will happen in two or three dimensions. In one dimension the memory function has inverse square root divergencies, because it is essentially given by the two-magnon density of states. In two dimensions we expect at most logarithmic divergencies. In three dimensions the memory function remains finite but it has a sharp structure with discontinuous derivatives.

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